Slides, notes, and exercises at:
https://github.com/cheshyre/nptls-hf

OAK RIDGE National Laboratory | LEADERSHIP COMPUTING FACILITY

Hartree-Fock calculations of nuclei

Nuclear Physics Turtle Lecture Series 2025:
Ab initio Hartree-Fock calculations of nuclei

Lecture 4

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Recap

- We have some V_{NN}, V_{3N}
- We know how to solve Hartree-Fock to optimize our basis
  - Iteratively build density matrix, build Fock operator, and diagonalize
- We need to identify a suitable starting basis that is convenient for nuclear structure

Main messages

- Harmonic oscillator is a **convenient starting point** for nuclear structure
- Standard ordering of levels (Bohr-Mottelson) to identify trial state $|\Phi_{\text{trial}}\rangle$
- Nuclear A-body Hamiltonian has a few complications
  - Notably: Subtraction of **center of mass**
- Finite basis size can lead to shortcomings
  - Need to test basis truncation and frequency $\hbar\omega$

HF for nuclei on whiteboard

Summary

- **Hartree-Fock for nuclei is same as before**
- Choose basis of **HO states**: $|p\rangle = |n(ls)jm_j m_t\rangle$
  - Energy ordering of states given by HO with spin-orbit splitting
  - **Test effect of finite basis size** by increasing truncation and varying $\hbar\omega$
- Many-body Hamiltonian needs to have **center of mass removed**
  - $H = T - T_{\mathrm{CM}} + V_{NN} + V_{3N}$